

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 09:58:14 ON 27 OCT 2008
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8  
 DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

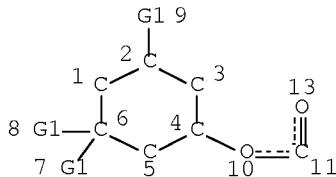
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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=> d sta que 114
L12          STR
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VAR G1=AK/ID
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
RSPEC 4
NUMBER OF NODES IS 12
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STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 527973 ITERATIONS          432 ANSWERS
SEARCH TIME: 00.00.07
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=> fil hcplus
FILE 'HCPLUS' ENTERED AT 09:58:28 ON 27 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 137 bib abs hitstr retable tot

L37	ANSWER 1 OF 8	HCAPLUS	COPYRIGHT 2008 ACS on STN			
AN	2005:96462	HCAPLUS	<u>Full-text</u>			
DN	142:161998					
TI	Cis-3,3,5-trimethylcyclohexyl esters for use as fragrances					
IN	Kuhn, Walter; Surburg, Horst					
PA	Symrise GmbH & Co. Kg, Germany					
SO	PCT Int. Appl., 33 pp.					
	CODEN: PIXXD2					
DT	Patent					
LA	German					
FAN.CNT	1					
	PATENT NO.	KIND	DATE	APPLICATION NO.		
PI	WO 2005009492	A1	20050203	WO 2004-EP51292		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		20040630	<--		
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
	DE 10332908	A1	20050210	DE 2003-10332908	20030719	<--
	EP 1648526	A1	20060426	EP 2004-741922	20040630	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
	US 20060211597	A1	20060921	US 2006-565241	20060119	<--
PRAI	DE 2003-10332908	A	20030719			
	WO 2004-EP51292	W	20040630			
OS	MARPAT 142:161998					

AB The invention relates to mixts. of cis-3,3,5-trimethylcyclohexyl esters with trans-3,3,5-trimethylcyclohexyl esters, the use of cis-3,3,5-trimethylcyclohexyl esters as fragrances and individual cis-3,3,5-trimethylcyclohexyl esters and their use as fragrances. Thus 3,3,5-trimethylcyclohexyl acetate was synthesized from 3,3,5-trimethylcyclohexanol and acetic acid anhydride; the product contained 90% cis-3,3,5-trimethylcyclohexyl acetate. It was used in a fragrance composition as 65 weight part ingredient; other components were (weight parts): benzyl acetate 30; Ozonil (2-Tridecennitrile) 10% in diethylphthalate 5; dihydromyrcenol 150; decanal 1; 2-phenoxyethylisobutyrate 100; methylcedrylketon 35; hexyl cinnamic aldehyde 50; Lilial 30; linalyl acetate 100; Galaxolide 50% in diethylphthalate 10; cedryl acetate 30; Zibeth absolute synth. 1; lemon terpene 70; ethylvanillin 3;  $\gamma$ -undecalactone 1; citronitril 10; Projasmon P (2-heptylcycloheptanon) 1; Agrumex HC (2-tert.-butylcyclohexyl acetate) 30; hexenyl isobutyrate, cis/trans- 1; hexenylacetate cis/trans- 1; Limette oil, synth. 10; diethylphthalate 2.66.

IT 828912-43-2P 828912-45-4P 828912-47-6P

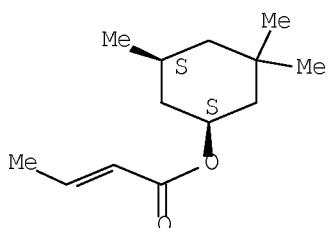
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)

RN 828912-43-2 HCAPLUS

CN 2-Butenoic acid, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

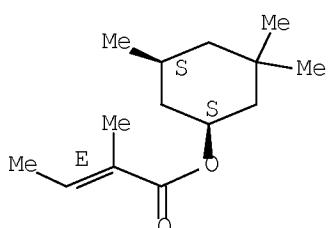


RN 828912-45-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester,  
(2E)-rel- (CA INDEX NAME)

Relative stereochemistry.

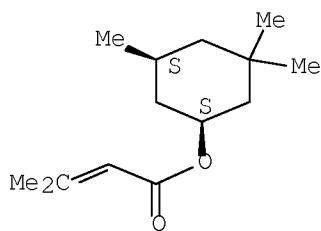
Double bond geometry as shown.



RN 828912-47-6 HCAPLUS

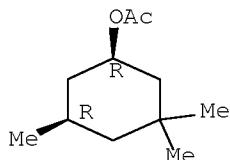
CN 2-Butenoic acid, 3-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

Relative stereochemistry.



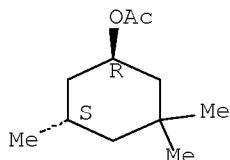
IT 24691-16-5P 24691-18-7P 60234-70-0P  
 60234-71-1P 828912-37-4P 828912-38-5P  
 828912-39-6P 828912-40-9P 828912-41-0P  
 828912-42-1P 828912-44-3P 828912-46-5P  
 828912-48-7P  
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)  
 RN 24691-16-5 HCPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



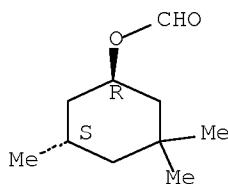
RN 24691-18-7 HCPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



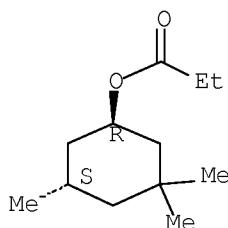
RN 60234-70-0 HCPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, formate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



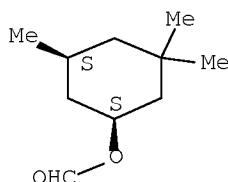
RN 60234-71-1 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, propanoate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



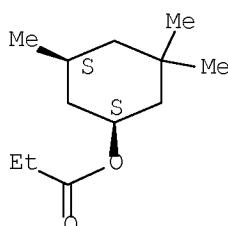
RN 828912-37-4 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-formate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 828912-38-5 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-propanoate, (1R,5R)-rel- (CA INDEX NAME)

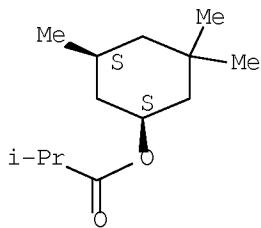
Relative stereochemistry.



RN 828912-39-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

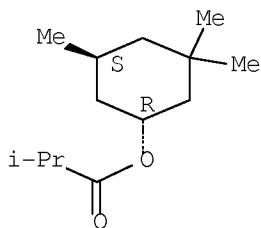
Relative stereochemistry.



RN 828912-40-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

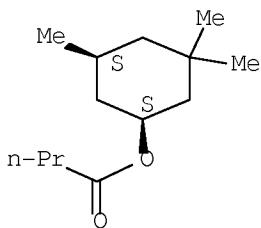
Relative stereochemistry.



RN 828912-41-0 HCAPLUS

CN Butanoic acid, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX  
NAME)

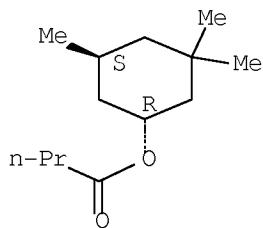
Relative stereochemistry.



RN 828912-42-1 HCAPLUS

CN Butanoic acid, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX  
NAME)

Relative stereochemistry.

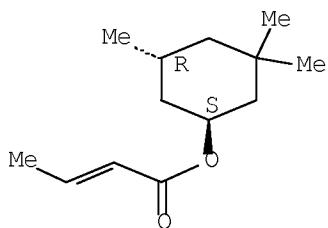


RN 828912-44-3 HCPLUS

CN 2-Butenoic acid, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

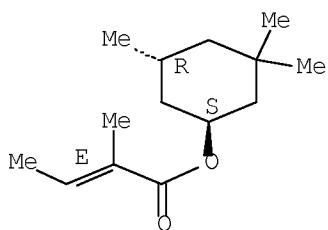


RN 828912-46-5 HCPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, (2E)-rel- (CA INDEX NAME)

Relative stereochemistry.

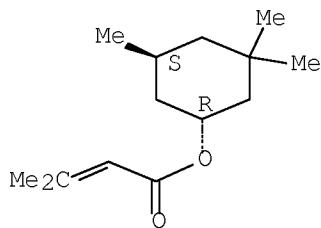
Double bond geometry as shown.



RN 828912-48-7 HCPLUS

CN 2-Butenoic acid, 3-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.



## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Henkel & Cie Gmbh	1976			DE 2518392 A	HCAPLUS
Merckle Kg Chem Pharm L	1974			DE 2326061 A	HCAPLUS
Poli Ind Chimica Spa	1974			DE 2406849 A	HCAPLUS
Rohde, U	2001			WO 0143784 A	HCAPLUS
Roussel-Uclaf	1970			DE 2026409 A	HCAPLUS

L37 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:423916 HCAPLUS Full-text

DN 137:6868

TI High-heat resistance low-hygroscopicity (meth)acrylic resins

IN Asada, Takeshi; Kakumoto, Satoru; Takahashi, Ikuo

PA Daicel Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

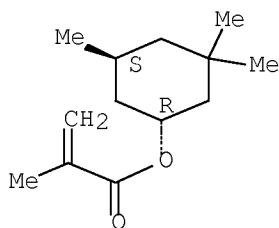
DT Patent

LA Japanese

FAN.CNT 1

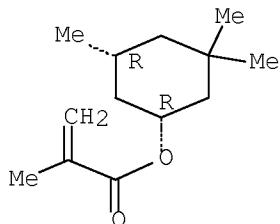
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002161112	A	20020604	JP 2000-361974	20001128 <--
PRAI	JP 2000-361974		20001128 <--		
AB Resins contain >3% trimethylcyclohexyl (meth)acrylate, which contains >50 mol% trans- or cis-isomer. Thus, trans-3,3,5-trimethylcyclohexyl methacrylate was prepared and polymerized with AIBN to prepare a polymer.					
IT 433334-69-1P 433334-70-4P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (trimethylcyclohexyl (meth)acrylate resins)					
RN 433334-69-1 HCAPLUS					
CN 2-Propenoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel-(CA INDEX NAME)					

Relative stereochemistry.



RN 433334-70-4 HCAPLUS  
 CN 2-Propenoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel-  
 (CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 AN 2001:452890 HCAPLUS Full-text  
 DN 135:66066  
 TI Ester odor neutralizers  
 IN Rohde, Ute; Hillers, Stephan; Surburg, Horst; Sonnenberg, Steffen; Mcdermott, Keith; Smith, Leslie; Sparkuhle, Karl  
 PA Haarmann & Reimer G.m.b.H., Germany; Haarmann und Reimer G.m.b.H.  
 SO PCT Int. Appl., 52 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001043784	A2	20010621	WO 2000-EP12374	20001208
	WO 2001043784	A3	20011115		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1239890	A2	20020918	EP 2000-991148	20001208
	EP 1239890	B1	20041110		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003516813	T	20030520	JP 2001-544920	20001208
	AT 281847	T	20041115	AT 2000-991148	20001208
	ES 2231305	T3	20050516	ES 2000-991148	20001208
	US 20030068295	A1	20030410	US 2002-149564	20020909
	US 7157411	B2	20070102		
PRAI	US 1999-170424P	P	19991213		
	WO 2000-EP12374	W	20001208		
OS	MARPAT 135:66066				
AB	This invention relates to odor neutralizers comprising esters such as 2,4-dimethyl-3-pentyl esters of propionic, isobutyric, crotonic, and butyric				

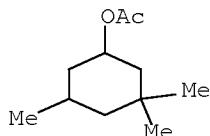
acids. These esters and a number of other similar esters were prepared and tested for their deodorant properties against sweat, ammonia, tobacco smoke, etc.

IT 67859-96-5P 94021-79-1P 94200-12-1P  
105937-88-0P 123232-56-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(ester odor neutralizers)

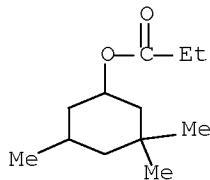
RN 67859-96-5 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



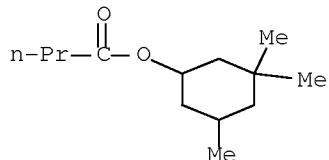
RN 94021-79-1 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-propanoate (CA INDEX NAME)



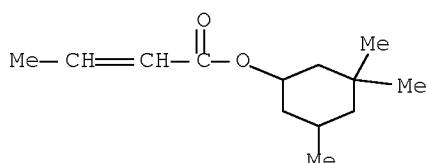
RN 94200-12-1 HCPLUS

CN Butanoic acid, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)

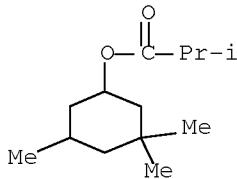


RN 105937-88-0 HCPLUS

CN 2-Butenoic acid, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)



RN 123232-56-4 HCAPLUS  
 CN Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester (CA INDEX  
 NAME)



L37 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:576823 HCAPLUS Full-text

DN 111:176823

OREF 111:29439a,29442a

TI Liquid detergent-bleach compositions containing perfume

IN Kishida, Koichi; Imanishi, Yoshitake

PA Taiyo Perfumery Co., Ltd., Japan

SO Jpn. Kokai Tokyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 01056798	A	19890303	JP 1987-213059	19870828 <--
PRAI JP 1987-213059		19870828		<--

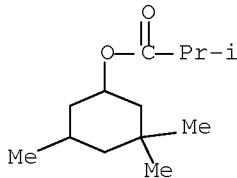
AB The compns., showing good odor-masking effects in the detergents and on laundered towels, contain hypochlorite 1-8 (as active Cl), alkali hydroxide 0.5-5, surfactant 0.1-5, and ≥1 of a list of selected perfumes 0.01-1%. A typical composition comprising NaOCl 6 (as active Cl), polyethylene glycol nonylphenyl ether sulfate Na salt 4, NaOH 3, campholenyl alc. 0.1, and water to 100% showed good odor masking, even after being stored 21 days at 45° in a polyethylene bottle.

IT 123232-56-4

RL: TEM (Technical or engineered material use); USES (Uses)  
 (perfumes, liquid laundry detergent-hypochlorite bleach compns. containing)

RN 123232-56-4 HCAPLUS

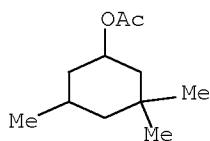
CN Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester (CA INDEX  
 NAME)



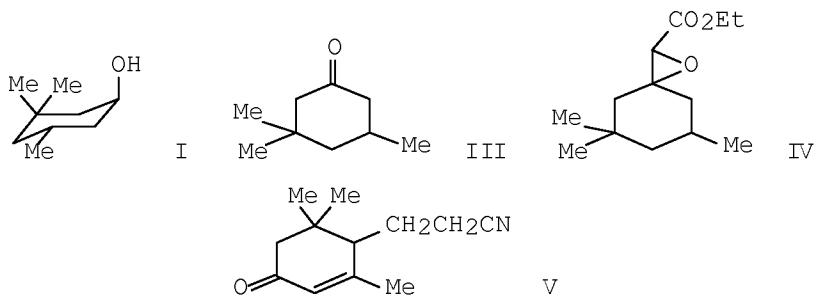
L37 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1986:33872 HCPLUS Full-text  
 DN 104:33872  
 OREF 104:5553a,5556a  
 TI Ultraviolet absorbing compounds and compositions containing these compounds  
 IN Baker, James Albert  
 PA Graesser Laboratories Ltd., UK  
 SO Eur. Pat. Appl., 25 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 153089 R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE GB 2155467 GB 2155467 US 4592906 AU 8538675 ZA 8501081 JP 60231637	A1 A B A A A A	19850828 19850925 19870325 19860603 19850822 19861029 19851118	EP 1985-300800 GB 1985-3039 US 1985-699955 AU 1985-38675 ZA 1985-1081 JP 1985-27539	19850206 <-- 19850206 <-- 19850208 <-- 19850213 <-- 19850213 <-- 19850214 <--
PRAI	GB 1984-3836	A	19840214	<--	
OS	MARPAT 104:33872				
AB	4-Me <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> CH:CHCO <sub>2</sub> R (I; R = 2-ethylhexyl, 2-octyl) were prepared for use as UV (type A) absorbers in sunscreen compns. Thus, 40 g I (R = Et), 60 mL 2-ethylhexanol, 60 mL PhMe, and 0.1 g Na were stirred at 130° to give, after workup and vacuum distillation, 38 g I (R = 2-ethylhexyl; II). II has a m.p. of -5°, is completely miscible with both mineral oil and MeOH, and has an absorptivity of 101 at λ <sub>max</sub> = 363 nm. Several sun-block formulations were given.				
IT	67859-96-5 RL: RCT (Reactant); RACT (Reactant or reagent) (condensation of, with dimethylaminobenzaldehyde)				
RN	67859-96-5 HCPLUS				
CN	Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)				



L37 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2008 ACS on STN  
 AN 1976:494493 HCPLUS Full-text  
 DN 85:94493  
 OREF 85:15145a,15148a  
 TI Synthesis of scented compounds from isophorone  
 AU Podlejski, Jerzy; Wilczynska, Janina  
 CS Inst. Fundam. Food Chem., Lodz Polytech Univ., Lodz, Pol.  
 SO Tluszcze, Srodk Piorace, Kosmetyki (1975), 19(12), 516-20  
 CODEN: TSPKBZ; ISSN: 0372-1795  
 DT Journal  
 LA Polish  
 GI



AB Trans-3,3,5-Trimethylcyclohexanol (I) was obtained in 90% yield from isophorone (II) by reduction with Raney Ni 15 hr at 95° and 40 atmospheric whereas II was reduced on Ni(HCO<sub>2</sub>)<sub>2</sub> at 60° to give 98% III. Dihydroisophorone condensed with ClCH<sub>2</sub>CO<sub>2</sub>Et in PhMe containing Na at 0° gave 65% IV which was hydrolyzed and decarboxylated to give 50% 1-formyl-3,3,5-trimethylcyclohexane. Condensation of II with MeCO<sub>2</sub>CMe:CH<sub>2</sub> followed by treatment with CH<sub>2</sub>:CHCN and hydrolysis gave 60% V useful as a scent for tobacco.

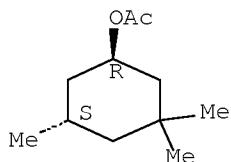
IT 24691-18-7P 60234-70-0P 60234-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 24691-18-7 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

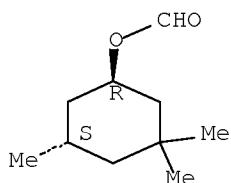
Relative stereochemistry.



RN 60234-70-0 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, formate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

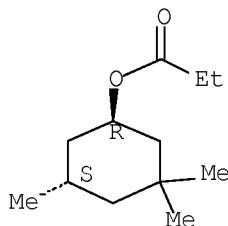
Relative stereochemistry.



RN 60234-71-1 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, propanoate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2008 ACS on STN

AN 1970:465956 HCPLUS Full-text

DN 73:65956

OREF 73:10799a,10802a

TI Reductions with metal-ammonia combinations. II. Monothioacetals and monothioketals. Synthesis of alkoxymercaptans

AU Eliel, Ernest L.; Doyle, Terrence W.

CS Dep. of Chem., Univ. of Notre Dame, Notre Dame, IN, USA

SO Journal of Organic Chemistry (1970), 35(8), 2716-22

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 73:65956

AB The reduction of oxathiolanes and oxathianes with metal-liquid NH<sub>3</sub> combinations gives rise to β- and γ-alkoxymercaptans. Twenty-six cases were studied; yields are good for all oxathianes and most oxathiolanes (except those with very simple 2-alkyl groups) when the metal is Ca.

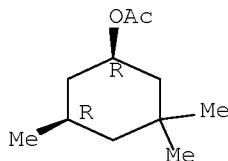
IT 24691-16-5P 24691-18-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 24691-16-5 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

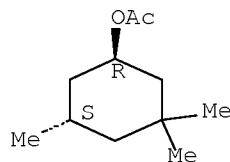
Relative stereochemistry.



RN 24691-18-7 HCPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2008 ACS on STN

AN 1968:29434 HCPLUS Full-text

DN 68:29434

OREF 68:5687a,5690a

TI 3,5,5-Trimethylcyclohexanol esters

IN Buzas, Andre

PA Laboratoires Bruneau et Cie.

SO Fr., 2 pp.

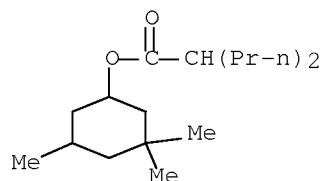
CODEN: FRXXAK

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1476627	-----	19670414	FR	19651220 <--
GI	For diagram(s), see printed CA Issue.				
AB	The preparation of esters of 3,5,5-trimethylcyclohexanol (I) which are of pharmacol. interest is described. I is treated either with the appropriate acid and a suitable catalyst, or with the corresponding acid chloride or anhydride in the presence of an amine e.g. pyridine. For example, I and m-(trifluoromethyl)phenyl- $\alpha$ -hydroxyacetic acid is refluxed in C <sub>2</sub> H <sub>4</sub> C <sub>12</sub> with 0.5% H <sub>2</sub> SO <sub>4</sub> for 7 hrs. The mixture is neutralized and the organic layer washed, dried, and distilled to give 85% 3,5,5-trimethylcyclohexyl m-(trifluoromethyl)phenyl- $\alpha$ - hydroxyacetate, m. 82°, b <sub>1</sub> 158°. Similarly prepared are the following II (R, % yield and phys. property given): m-F <sub>3</sub> CC <sub>6</sub> H <sub>4</sub> OCH <sub>2</sub> , 60, b <sub>20</sub> 193°; Pr <sub>2</sub> CH, 82, b <sub>25</sub> 165-7°; p-ClC <sub>6</sub> H <sub>4</sub> OCH <sub>2</sub> , 90, m. 92°.				
IT	17564-82-8P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	17564-82-8 HCPLUS				
CN	Valeric acid, 2-propyl-, 3,3,5-trimethylcyclohexyl ester (8CI) (CA INDEX NAME)				



=> => d his

(FILE 'HOME' ENTERED AT 09:41:15 ON 27 OCT 2008)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:41:30 ON 27 OCT 2008

L1           1 S US20060211597/PN OR (US2006-565241# OR WO2004-EP51292 OR DE20  
              E SYMRISE/CO

L2           329 S E3-E23/CO,PA,CS  
              E E15+ALL

L3           1136 S E2+RT OR E2-E28/CS,PA  
              E KUHN/AU

L4           11 S E3  
              E KUHN W/AU

L5           550 S E3-E14,E16-E20  
              E KUEHN/AU

L6           2 S E3  
              E KUEHN W/AU

L7           192 S E3-E6,E8-E9  
              E KEUHN/AU  
              E SURBURG/AU

L8           79 S E4,E6  
              E SUERBURG/AU

L9           1 S L1 AND L2-L8  
              SEL RN

FILE 'REGISTRY' ENTERED AT 09:44:04 ON 27 OCT 2008

L10          22 S E1-E22

L11          16 S L10 AND 46.150.1/RID AND O>=2

L12          STR

L13          1 S L12 CSS SAM

L14          432 S L12 CSS FUL  
              SAV TEMP L14 GRES0565A/A

L15          274 S L14 NOT STEREO?/FS

L16          58 S L15 AND 1/NC AND 3/ELC.SUB

L17          23 S L16 AND 1/NR

L18          13 S L17 AND 2/O

L19          11 S L18 NOT PMS/CI

L20          158 S L14 NOT L15

L21          28 S L20 AND 1/NC AND 3/ELC.SUB AND 1/NR

L22          12 S L21 NOT L11

L23          5 S L22 AND 2/O

L24          3 S L23 NOT PMS/CI

L25          30 S L11,L19,L24  
              SAV TEMP L25 GRES0565B/A

FILE 'HCAPLUS' ENTERED AT 09:51:25 ON 27 OCT 2008

L26          51 S L25

L27          2 S L26 AND L1-L9

L28          8 S L26 AND PY<=2004 NOT P/DT

L29          27 S L26 AND (PD<=20040630 OR PRD<=20040630 OR AD<=20040630) AND P

L30          35 S L28,L29

L31          3 S L30 AND L11

L32          4 S L27,L31

L33          1 S L30 AND L24

L34          5 S L32,L33

L35          30 S L30 NOT L34  
              SEL AN 16 19 21

L36          3 S L35 AND E23-E28

L37          8 S L34,L36

FILE 'REGISTRY' ENTERED AT 09:58:14 ON 27 OCT 2008

FILE 'HCAPLUS' ENTERED AT 09:58:28 ON 27 OCT 2008

SEL RN 3 L37

FILE 'REGISTRY' ENTERED AT 09:59:41 ON 27 OCT 2008

L38            42 S E29-E70  
L39            37 S L38 NOT L25  
L40            0 S L39 AND L14

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